

# Pore Collapse and Hot Spots in HMX

Ralph Menikoff, T-14

The computing power now available has led researchers to reconsider mesoscale simulations as a means to develop a detailed understanding of detonation waves in a heterogeneous explosive. Since chemical reaction rates are sensitive to temperature, hot spots are of critical importance for initiation. In a plastic bonded explosive, pore collapse is thought to be the dominant hot spot mechanism for shock initiation. Here, for the collapse of a single pore driven by a shock, the dependence of the temperature distribution on numerical resolution and dissipative mechanism is investigated. An inert material (with the constitutive properties of HMX) is used to better focus on the mechanics of pore collapse. Two important findings result from this study. First, too low a resolution can significantly enhance the hot spot mass. Second, at low piston velocities ( $< 1 \text{ km/s}$ ), shock dissipation alone does not generate sufficient hot spot mass. Two other dissipative mechanism investigated are plastic work and viscous heating. In the cases studied, the integrated temperature distribution has a power-law tail with slope related to a parameter with dimensions of viscosity. For a particular case, the parameter of either dissipative mechanism can be fit to obtain quantitatively the hot spot mass needed for initiation. But the dissipative mechanisms scale differently with shock strength and pore size. Consequently, to predict initiation behavior over a range of stimuli and as the micro-structure properties of a PBX are varied, sufficient numerical resolution and the correct physical dissipative mechanism are essential.

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ADC reviewed by Paul J. Dotson, T-DO

# **Pore Collapse and Hot Spots in HMX**

RALPH MENIKOFF, T-14

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# Shock Driven Pore Collapse

- Initial configuration

- Materials

- Boundary conditions

- Resolution

- Code

# Hot Spot Ignition

Reaction rates are very sensitive to temperature

Dependence of Temperature Distribution on the following:

- Shock strength

- Dissipation

- Pore size

- Geometry

- Resolution

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## Caveats

Thermal properties not accurately modeled

# Shock-to-Detonation Transition

- Temperature dependence
- Pressure dependence

## Implication

For sub micro-second time scale of SDT

Need hot-spot temperature  $\gtrsim 1000$  K

# Estimates based on Shock Hugoniot

## Hot Spot Temperature

- Impedance match, HMX → gas  
Jet velocity  $\approx 2 \times$  (piston velocity)
- Convergence effect  
Tip of jet  $\times 2$ , roughly
- Stagnation of jet  
Riemann problem, jet → ambient HMX

## Gas Temperature

- Gas adiabat  
Shock to  $u_p = 2 \times$  (piston velocity)
- Isentropic compression  
Up to stagnation pressure of jet

# Stages of Pore Collapse

Shock overtaking pore

Implosion phase

jet forms  
outward rarefaction

Explosion phase

jet stagnates and forms vortex  
outward shock & Mach node

Shock past pore

## Jet Formation

density  
scale: 1 to 3

velocity  
scale: 0 to 5

initial pore,  $0.3 < x < 0.5$   
piston velocity = 1.3

Surface velocity  $2 \times u_p$   
 $0.2 < x < 0.4$

Jet tip at pore center  
 $0.3 < x < 0.5$

Jet tip accelerates  
 $0.3 < x < 0.5$

Jet tip velocity  $4 \times u_p$   
 $0.35 < x < 0.55$

# Temperature after Pore Collapse

Blue region corresponds to  
compressed gas  
Vortex & gas interface  
are unstable  
Numerical artifacts  
Peak T at pore interface

Normalization  
mass of HMX in pore volume  
 $0.001 \approx 15$  cells  
 $\text{@} 100$  cells/pore radius  
Straight line on log-log plot  
implies power-law distribution

# Mesh Resolution

Piston velocity = 1.3 km/s

Hydro collapse

shock dissipation only

- Pressure

- Temperature

## Implication

Tail of temperature distribution  
is sensitive to resolution

# Plastic Dissipation

# Compare Dissipation

Hydro

Plastic,  $\eta = 80$  Poise

Viscous,  $\eta = 10$  Poise

## Results

Hi piston velocity = 1.3 km/s

Low piston velocity = 0.5 km/s

- Resolution

- Dissipation

- Geometry

### Implication

Tail of temperature distribution  
is sensitive to resolution & dissipative mechanism

## Comments & Questions

- Dissipation matters !  
Pure hydro not sufficient at low velocity.  
Pore size affects sensitivity (scaling)
- Power-law temperature distribution  
Physical or numerical artifact ?

————— future direction ————

- Pore collapse with reaction  
Mass reacted before hot spot quenches ?  
Volume burn or burn front ?  
Resolve combustion wave or subgrid model ?
- Distribution of pores  
(1% porosity  $\Rightarrow R/L \approx 0.2$  in 3-dimensions)  
Interaction of hot spots ?  
Coupling of energy release to lead shock ?